



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:04 AM UTC

PDB ID : 7I2S / pdb_00007i2s
Title : Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with Z31721798 (DNV2_NS5A-x0771)
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Deposited on : 2025-03-06
Resolution : 1.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

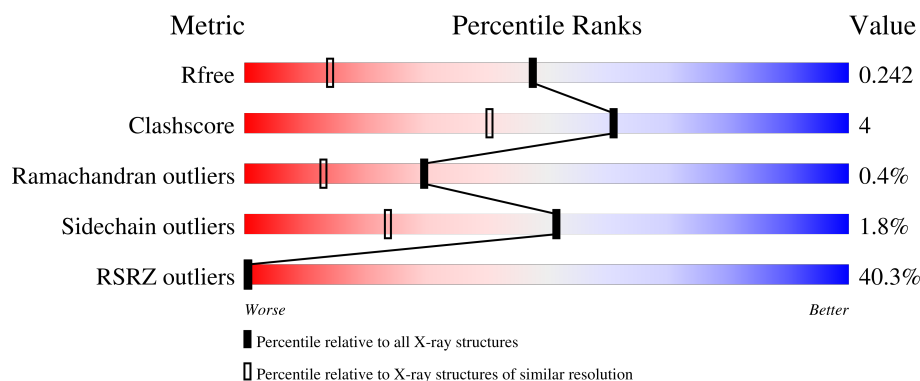
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	637	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	A	1008	-	-	X	-
7	NW4	A	1011	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5255 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	7	0
			4757	2994	853	876	34			

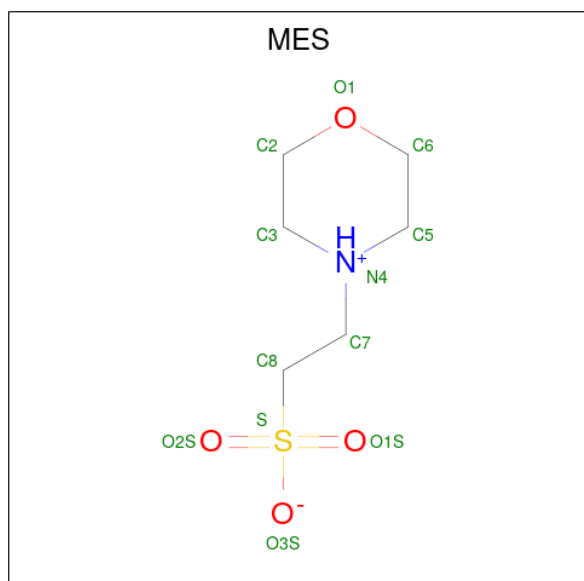
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



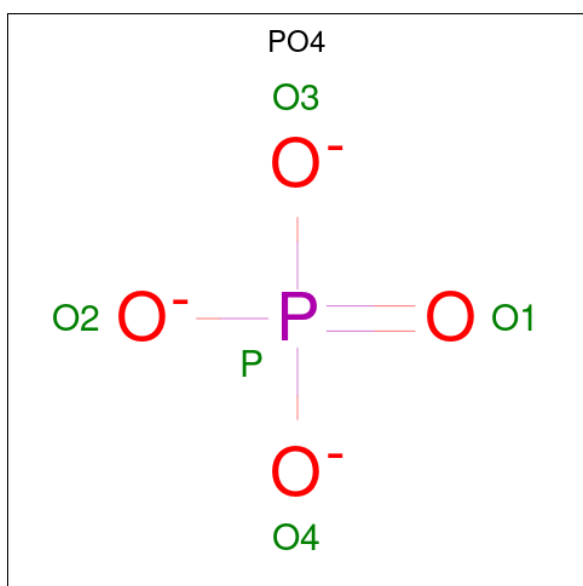
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



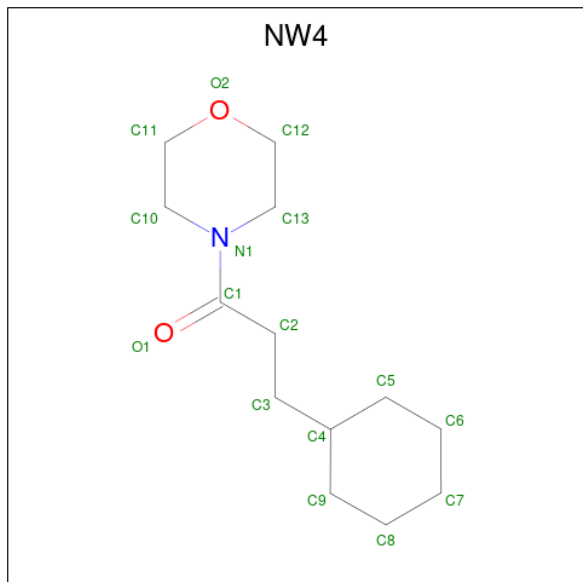
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is 3-cyclohexyl-1-(morpholin-4-yl)propan-1-one (CCD ID: NW4) (formula: $C_{13}H_{23}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			16	13	1	2		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

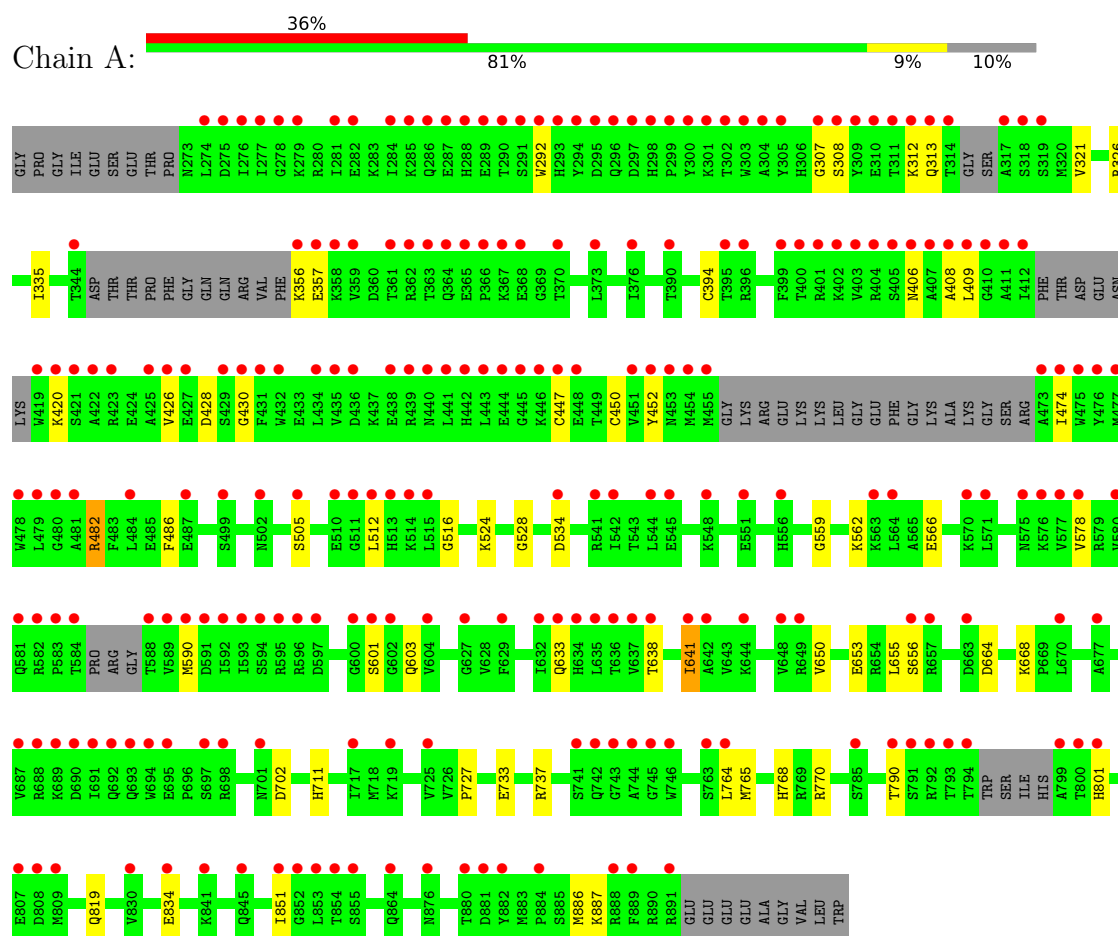
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	419	Total	O	0	0
			419	419		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NS5 RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.44Å 116.67Å 148.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 1.56 49.97 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.97-1.56) 99.5 (49.97-1.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.211 0.222 , 0.242	Depositor DCC
R_{free} test set	5192 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5255	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CL, DMS, NW4, ZN, MES, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	3/4862 (0.1%)	1.26	4/6557 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	N-CA	5.58	1.50	1.46
1	A	516	GLY	C-O	5.07	1.29	1.23
1	A	768	HIS	CE1-NE2	5.01	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	650	VAL	CA-C-O	-6.30	114.55	119.46
1	A	559	GLY	CA-C-N	5.16	127.97	120.79
1	A	559	GLY	C-N-CA	5.16	127.97	120.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4757	0	4660	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	3	0
5	A	14	0	20	0	0
6	A	10	0	0	4	0
7	A	16	0	0	0	0
8	A	1	0	0	0	0
9	A	419	0	0	10	2
All	All	5255	0	4724	40	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASP:OD1	6:A:1008:PO4:O4	1.90	0.88
4:A:1004:DMS:H11	9:A:1272:HOH:O	1.75	0.87
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.43	0.77
4:A:1004:DMS:H12	9:A:1328:HOH:O	1.91	0.70
1:A:428:ASP:OD1	1:A:430:GLY:N	2.30	0.65
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.12	0.64
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.17	0.63
1:A:733:GLU:O	1:A:737:ARG:HG3	1.99	0.62
1:A:409:LEU:O	1:A:482:ARG:HG2	2.00	0.61
1:A:638:THR:HA	1:A:641:ILE:CG2	2.30	0.61
1:A:534:ASP:OD1	6:A:1008:PO4:P	2.60	0.59
1:A:562:LYS:NZ	9:A:1108:HOH:O	2.35	0.59
1:A:834:GLU:HG3	9:A:1152:HOH:O	2.04	0.57
1:A:790:THR:HG22	9:A:1367:HOH:O	2.07	0.55
1:A:801[B]:HIS:H	1:A:801[B]:HIS:CD2	2.24	0.54
1:A:819:GLN:NE2	9:A:1107:HOH:O	2.34	0.50
1:A:653:GLU:O	1:A:656:SER:OG	2.23	0.50
4:A:1004:DMS:C1	9:A:1272:HOH:O	2.48	0.50
1:A:528:GLY:O	1:A:668:LYS:HE3	2.14	0.48
1:A:524:LYS:NZ	9:A:1118:HOH:O	2.47	0.48
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.47
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.16	0.46
1:A:764:LEU:HG	1:A:765:MET:CE	2.45	0.46
1:A:505:SER:OG	1:A:655:LEU:O	2.24	0.46
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.51	0.45
1:A:638:THR:O	1:A:641:ILE:HG23	2.16	0.45
1:A:512[A]:LEU:HG	1:A:727:PRO:HB3	1.99	0.44
1:A:452:TYR:HB2	1:A:578:VAL:HG22	2.00	0.43
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.49	0.42
1:A:292:TRP:CZ2	1:A:307:GLY:HA3	2.55	0.42
1:A:308:SER:HA	1:A:590:MET:O	2.20	0.42
1:A:408:ALA:HB3	1:A:603:GLN:HE22	1.84	0.42
1:A:409:LEU:HD22	9:A:1515:HOH:O	2.20	0.42
1:A:408:ALA:HB3	1:A:603:GLN:NE2	2.35	0.42
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.51	0.41
1:A:312:LYS:O	1:A:313:GLN:HG3	2.21	0.41
1:A:428:ASP:OD1	1:A:428:ASP:C	2.63	0.41
1:A:638:THR:HA	1:A:641:ILE:HG22	2.03	0.41
1:A:886:MET:HE1	9:A:1155:HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1162:HOH:O	9:A:1162:HOH:O[2_445]	1.56	0.64
9:A:1292:HOH:O	9:A:1415:HOH:O[2_545]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	569/637 (89%)	551 (97%)	16 (3%)	2 (0%)	30 13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	420	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	511/554 (92%)	502 (98%)	9 (2%)	51 24

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	LYS
1	A	357	GLU
1	A	426	VAL
1	A	474	ILE
1	A	482	ARG
1	A	601	SER
1	A	633	GLN
1	A	641	ILE
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	575	ASN
1	A	603	GLN
1	A	618	GLN
1	A	705	GLN
1	A	868	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	DMS	A	1006	-	3,3,3	0.25	0	3,3,3	0.42	0
3	MES	A	1003[A]	-	12,12,12	0.73	0	15,16,16	0.94	1 (6%)
6	PO4	A	1008	-	4,4,4	6.15	3 (75%)	6,6,6	0.95	0
6	PO4	A	1009	-	4,4,4	1.33	1 (25%)	6,6,6	0.49	0
4	DMS	A	1004	-	3,3,3	0.95	0	3,3,3	0.65	0
5	PEG	A	1007	-	6,6,6	0.21	0	5,5,5	0.18	0
4	DMS	A	1005	-	3,3,3	0.33	0	3,3,3	0.05	0
7	NW4	A	1011	-	17,17,17	0.18	0	21,21,21	0.59	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.32	0
5	PEG	A	1010	-	6,6,6	0.14	0	5,5,5	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
5	PEG	A	1007	-	-	1/4/4/4	-
7	NW4	A	1011	-	-	4/9/25/25	0/2/2/2
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	1010	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	9.00	1.71	1.50
6	A	1008	PO4	P-O2	6.70	1.74	1.54
6	A	1008	PO4	P-O3	4.90	1.68	1.54
6	A	1009	PO4	P-O1	2.30	1.56	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003[A]	MES	O2S-S-C8	-2.04	103.64	106.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

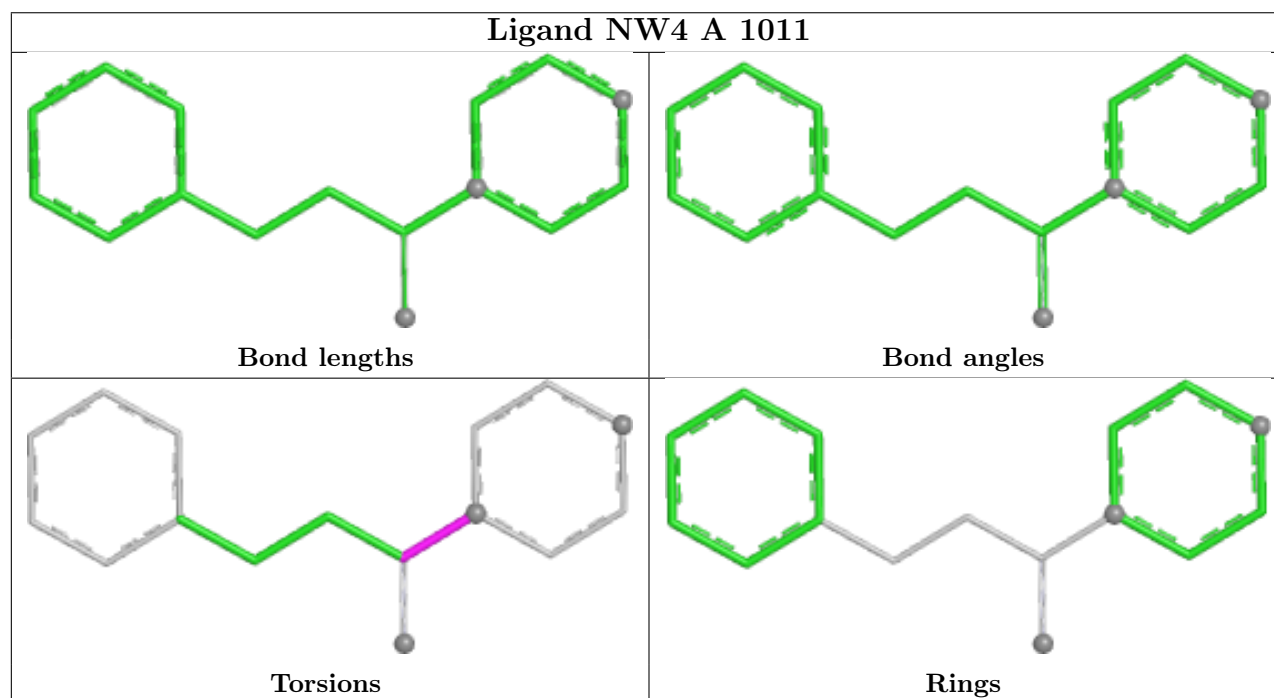
Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O2S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1011	NW4	O1-C1-N1-C10
7	A	1011	NW4	C2-C1-N1-C10
7	A	1011	NW4	C2-C1-N1-C13
7	A	1011	NW4	O1-C1-N1-C13
5	A	1010	PEG	O2-C3-C4-O4
5	A	1007	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1010	PEG	O1-C1-C2-O2
5	A	1010	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1008	PO4	4	0
4	A	1004	DMS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	576/637 (90%)	2.65	232 (40%) 0 0	5, 32, 85, 127	99 (17%)

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	851	ILE	16.0
1	A	853	LEU	14.6
1	A	303	TRP	13.9
1	A	512[A]	LEU	13.7
1	A	451	VAL	13.4
1	A	593	ILE	13.3
1	A	478	TRP	13.3
1	A	592	ILE	13.2
1	A	636	THR	12.8
1	A	725	VAL	12.6
1	A	515	LEU	12.6
1	A	635	LEU	12.6
1	A	426	VAL	12.5
1	A	304	ALA	12.4
1	A	475	TRP	12.4
1	A	852	GLY	12.3
1	A	801[A]	HIS	12.3
1	A	419	TRP	12.0
1	A	855	SER	11.3
1	A	589	VAL	11.2
1	A	854	THR	11.0
1	A	409	LEU	10.7
1	A	412	ILE	10.5
1	A	719[A]	LYS	10.5
1	A	400	THR	10.5
1	A	476	TYR	9.8
1	A	411	ALA	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	431	PHE	9.6
1	A	292	TRP	9.5
1	A	511	GLY	9.4
1	A	317	ALA	9.3
1	A	513	HIS	9.3
1	A	841	LYS	9.1
1	A	594	SER	9.1
1	A	888	ARG	9.0
1	A	363	THR	9.0
1	A	697	SER	8.9
1	A	473	ALA	8.9
1	A	575	ASN	8.7
1	A	576	LYS	8.7
1	A	743	GLY	8.6
1	A	453	ASN	8.5
1	A	845	GLN	8.5
1	A	356	LYS	8.5
1	A	499	SER	8.4
1	A	477	MET	8.4
1	A	402	LYS	8.4
1	A	410	GLY	8.4
1	A	763[A]	SER	8.3
1	A	505	SER	8.3
1	A	584	THR	8.3
1	A	601	SER	8.3
1	A	656	SER	8.2
1	A	785[A]	SER	8.1
1	A	588	THR	8.1
1	A	454	MET	8.1
1	A	302	THR	8.1
1	A	474	ILE	8.1
1	A	590	MET	7.9
1	A	591	ASP	7.8
1	A	408	ALA	7.7
1	A	808	ASP	7.7
1	A	864[A]	GLN	7.7
1	A	401	ARG	7.6
1	A	514	LYS	7.6
1	A	421	SER	7.6
1	A	657	ARG	7.5
1	A	649	ARG	7.5
1	A	298	HIS	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	405	SER	7.4
1	A	396	ARG	7.3
1	A	595	ARG	7.3
1	A	309	TYR	7.3
1	A	359	VAL	7.3
1	A	319	SER	7.3
1	A	318	SER	7.1
1	A	284	ILE	7.0
1	A	809	MET	7.0
1	A	299	PRO	6.9
1	A	741[A]	SER	6.9
1	A	600	GLY	6.8
1	A	689	LYS	6.8
1	A	403	VAL	6.8
1	A	698	ARG	6.7
1	A	541	ARG	6.7
1	A	583	PRO	6.7
1	A	502	ASN	6.6
1	A	548	LYS	6.6
1	A	510	GLU	6.5
1	A	404	ARG	6.5
1	A	688	ARG	6.4
1	A	290	THR	6.3
1	A	551	GLU	6.3
1	A	807	GLU	6.3
1	A	294	TYR	6.2
1	A	406	ASN	6.2
1	A	487	GLU	6.1
1	A	693	GLN	5.9
1	A	358	LYS	5.8
1	A	597	ASP	5.8
1	A	455	MET	5.7
1	A	420	LYS	5.7
1	A	596	ARG	5.6
1	A	407	ALA	5.5
1	A	441	LEU	5.4
1	A	365	GLU	5.4
1	A	742	GLN	5.3
1	A	314	THR	5.3
1	A	690	ASP	5.2
1	A	277	ILE	5.2
1	A	357	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	692	GLN	5.1
1	A	281	ILE	5.1
1	A	297	ASP	5.0
1	A	637	VAL	5.0
1	A	305	TYR	4.9
1	A	435	VAL	4.8
1	A	308	SER	4.8
1	A	364	GLN	4.7
1	A	422	ALA	4.7
1	A	799	ALA	4.7
1	A	442	HIS	4.6
1	A	361	THR	4.5
1	A	362	ARG	4.5
1	A	434	LEU	4.5
1	A	301	LYS	4.4
1	A	794	THR	4.3
1	A	571	LEU	4.3
1	A	791	SER	4.3
1	A	436	ASP	4.2
1	A	427	GLU	4.1
1	A	432	TRP	4.1
1	A	793	THR	4.1
1	A	278	GLY	4.0
1	A	274	LEU	4.0
1	A	300	TYR	3.9
1	A	452	TYR	3.9
1	A	279	LYS	3.8
1	A	445	GLY	3.8
1	A	479	LEU	3.8
1	A	293	HIS	3.8
1	A	484	LEU	3.8
1	A	448	GLU	3.8
1	A	694	TRP	3.7
1	A	370	THR	3.7
1	A	288	HIS	3.7
1	A	880	THR	3.6
1	A	790	THR	3.6
1	A	889	PHE	3.6
1	A	295	ASP	3.6
1	A	443	LEU	3.5
1	A	564	LEU	3.5
1	A	641	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	481	ALA	3.5
1	A	344	THR	3.5
1	A	891	ARG	3.4
1	A	276	ILE	3.3
1	A	744	ALA	3.3
1	A	366	PRO	3.3
1	A	275	ASP	3.3
1	A	577	VAL	3.3
1	A	746	TRP	3.2
1	A	423	ARG	3.2
1	A	544	LEU	3.2
1	A	638	THR	3.2
1	A	311	THR	3.2
1	A	376	ILE	3.1
1	A	296	GLN	3.1
1	A	291	SER	3.1
1	A	399	PHE	3.1
1	A	792	ARG	3.1
1	A	287	GLU	3.0
1	A	881	ASP	3.0
1	A	313	GLN	3.0
1	A	745	GLY	3.0
1	A	425	ALA	2.9
1	A	677	ALA	2.9
1	A	629	PHE	2.8
1	A	670	LEU	2.8
1	A	634	HIS	2.8
1	A	627	GLY	2.7
1	A	800	THR	2.7
1	A	289	GLU	2.7
1	A	286	GLN	2.7
1	A	580	VAL	2.7
1	A	480	GLY	2.7
1	A	582	ARG	2.7
1	A	563	LYS	2.6
1	A	312	LYS	2.6
1	A	438	GLU	2.6
1	A	439	ARG	2.6
1	A	444	GLU	2.6
1	A	545	GLU	2.6
1	A	282	GLU	2.5
1	A	581	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	447	CYS	2.5
1	A	430	GLY	2.5
1	A	648	VAL	2.5
1	A	307	GLY	2.4
1	A	632	ILE	2.4
1	A	429	SER	2.4
1	A	644	LYS	2.4
1	A	882	TYR	2.4
1	A	368	GLU	2.4
1	A	570	LYS	2.3
1	A	691	ILE	2.3
1	A	764	LEU	2.3
1	A	534	ASP	2.3
1	A	285	LYS	2.3
1	A	310	GLU	2.3
1	A	542	ILE	2.3
1	A	633	GLN	2.3
1	A	876	ASN	2.3
1	A	390	THR	2.3
1	A	663	ASP	2.2
1	A	395	THR	2.2
1	A	642	ALA	2.1
1	A	717	ILE	2.1
1	A	556	HIS	2.1
1	A	578	VAL	2.1
1	A	695	GLU	2.1
1	A	687	VAL	2.1
1	A	446	LYS	2.1
1	A	440	ASN	2.1
1	A	602	GLY	2.1
1	A	701	ASN	2.1
1	A	884	PRO	2.1
1	A	367	LYS	2.0
1	A	830	VAL	2.0
1	A	373	LEU	2.0
1	A	834	GLU	2.0
1	A	604	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

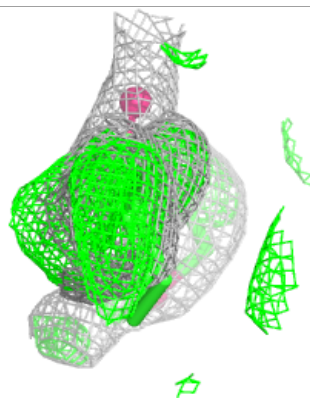
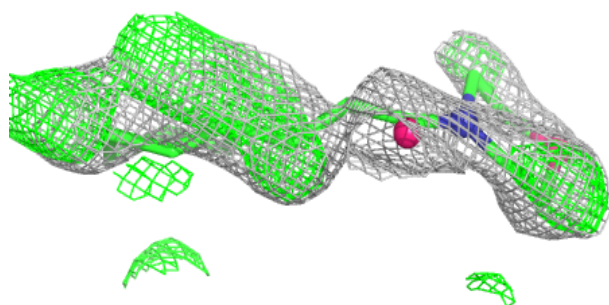
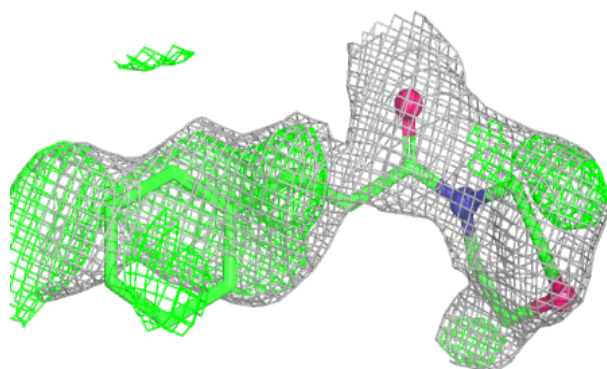
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NW4	A	1011	16/16	0.59	0.45	44,46,47,48	16
6	PO4	A	1009	5/5	0.61	0.19	69,70,89,105	0
4	DMS	A	1005	4/4	0.68	0.27	63,78,86,96	0
5	PEG	A	1007	7/7	0.71	0.18	65,72,84,85	0
6	PO4	A	1008	5/5	0.75	0.17	30,32,42,60	0
5	PEG	A	1010	7/7	0.82	0.18	62,69,73,74	0
4	DMS	A	1004	4/4	0.90	0.16	36,38,40,41	0
4	DMS	A	1006	4/4	0.95	0.12	43,46,51,54	0
3	MES	A	1003[A]	12/12	0.97	0.33	18,22,24,24	12
3	MES	A	1003[B]	12/12	0.97	0.33	483,499,513,515	12
2	ZN	A	1002	1/1	0.98	0.07	47,47,47,47	0
8	CL	A	1012	1/1	0.99	0.06	36,36,36,36	0
2	ZN	A	1001	1/1	1.00	0.01	18,18,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NW4 A 1011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.